When Lethal Agents Rain from the Sky

CONSIDER this: a ballistic missile carrying a chemical or biological agent is traveling fast toward its target—military or otherwise. What are the implications of intercepting or destroying that missile in the upper atmosphere?

Part of the answer to that question depends on knowing what conditions would allow lethal amounts of the liquid agent to reach the ground.

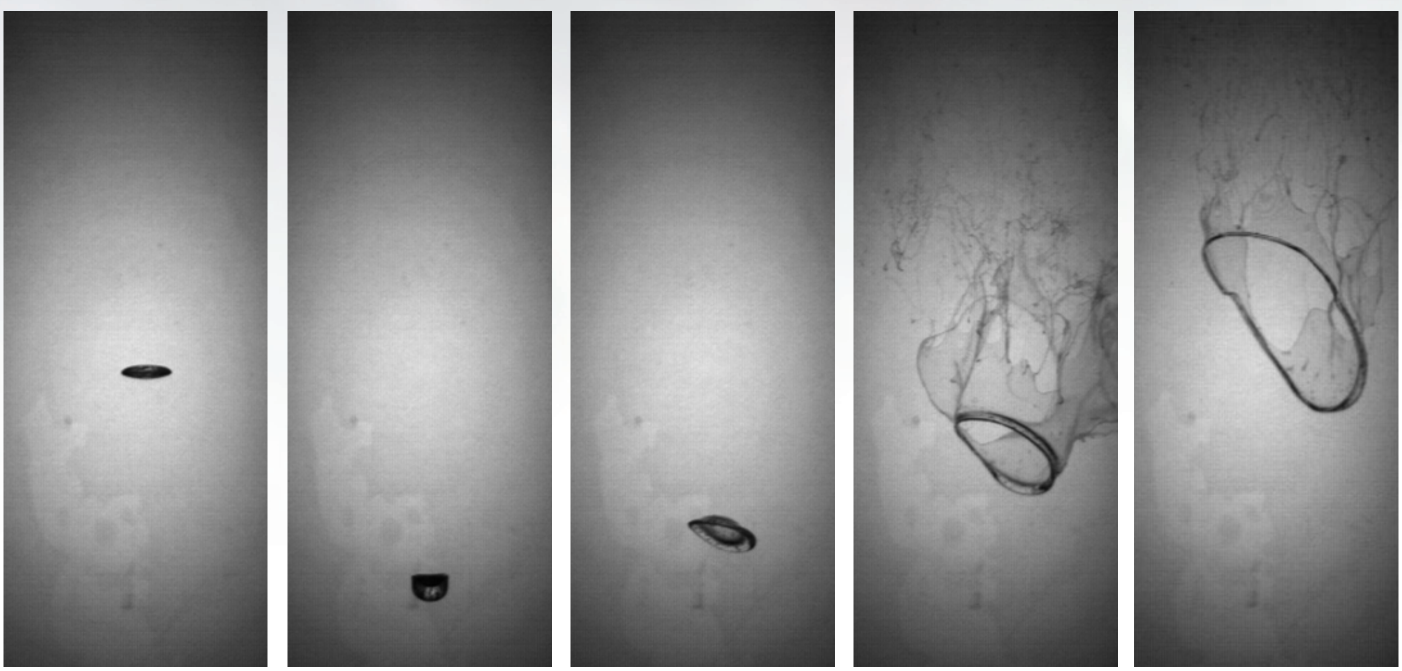
For instance, consider the chemical nerve agent VX, an organophosphorous compound that disrupts the body's nervous system. Lethal doses—ingested, inhaled, or absorbed through the skin—cause rapid death. It is estimated that a lethal dose is contained in a 2- to 3-millimeter-size drop. A warhead holding 400 kilograms of VX contains about 62 million lethal doses. If the warhead were to reach its target—say, a port or air base—it would saturate the target and cause an "area denial," that is, make the target site unusable until cleaned up. But what if it were to be intercepted tens of kilometers above the ground? What would happen to the VX?

The extreme conditions experienced by a single liquid drop during its reentry into the atmosphere lie in a regime for which no experimental data exist. To better understand the physics of what happens at these altitudes, physicist Glen Nakafuji, analyst Roxana Greenman, professor Theo Theafanous of the University of California (UC) at Santa Barbara, and research colleagues are studying how liquid breaks up and evolves in rarefied (thin) atmospheres.

To do so, they are using unique hydrodynamic and shock-physics experiments coupled with advanced chemical–kinetic and hydrodynamics computer codes. The experiments and codes simulate the supersonic, rarefied flow environments that reentering droplets of a chemical agent would experience. Nakafuji is the principal investigator for the project, which is funded by the Laboratory Directed Research and Development (LDRD) Program.

Thin Atmospheres, High Velocities, Surface Tension

A number of complicated factors determine how a body of liquid breaks up and how the individual drops or streamers break



Series of photos showing "bag breakup" of a liquid drop, in which the round drop deforms into a shape resembling a bowler hat.

apart and shape and reshape themselves. The factors include the pressure of the surrounding atmosphere, the velocity at which the liquid is traveling, and the physical properties of the liquid. "At altitudes of tens of kilometers," explains Nakafuji, "the agent disperses and expands in an atmospheric pressure that can be ten thousand times less than that at sea level. Pieces of liquid float out, stretch, and tear in milliseconds, then fall in an expanding cloud into the atmosphere." From there, the mass of drops falls through the air, moving at supersonic velocities through increasing atmospheric pressure. "Originally," notes Nakafuji, "people in the field theorized that the liquid would aerosolize into droplets on the order of 10 micrometers in diameter and disperse. Initial experiments indicate that this may not be true." So the question remains open: Would a given liquid break up into these small-size droplets or not?

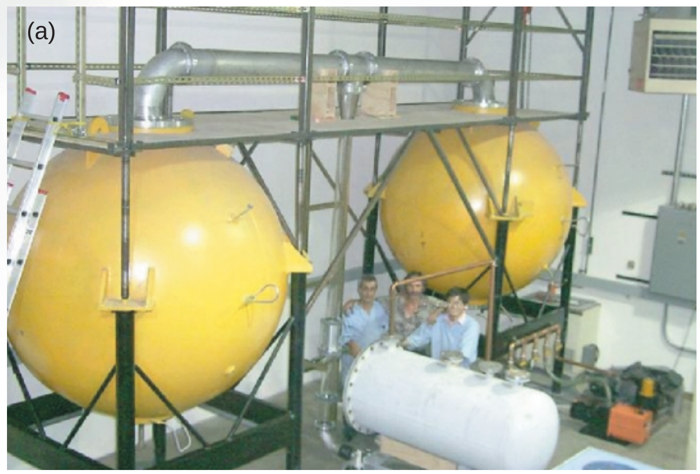
"There's a huge gap in experimental data for the behavior of liquids in this sort of environment," notes Nakafuji. "We know how various liquids break up at sea level, where the atmosphere is dense, and the air molecules—which can be represented as individual particles—are constantly bouncing off each other, pressing together, and acting more like a fluid than individual particles." However, higher up in the atmosphere, the molecules are fewer and more widely dispersed, acting more like individual particles at altitudes above 30 kilometers. "You add to this the fact that the liquid agent is not in free fall but is experiencing atmospheric drag, and the problem becomes very complex," notes Nakafuji. "Yet this is the situation we're faced with in examining the physics of droplet breakup."

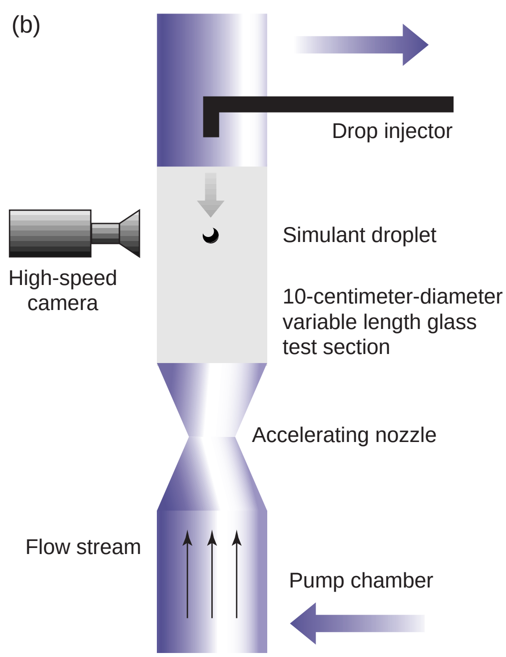
Of Weber Numbers and Bag Breakups

The physics of a liquid drop breaking up has much to do with the nature of the fluid (its density and viscosity, for instance) and the forces acting upon it. The ratio of external aerodynamic force—which tends to pull the drop apart—to the liquid's surface tension—which tends to hold the drop together—is a dimensionless quantity called the Weber number. Drops with different Weber numbers break up in different ways. Drops with higher Weber numbers (above 100) tend to have more catastrophic breakup and result in smaller drops. At very high altitudes, where external aerodynamic forces are small, the Weber number remains relatively low, below 100. When the team conducted experiments on drops with a range of Weber numbers characteristic of high altitudes, interesting findings emerged. For instance, drops 3 to 4 millimeters in diameter tended to oscillate before breakup. For drops with Weber numbers between 12 and 100, the experimenters observed a phenomenon called "bag breakup," in which a round drop deforms into a shape resembling a bowler hat, with a flat rim and curved crown. As the drop falls, the bag portion, which corresponds to the crown of the hat, oscillates in and out. When the original drop disintegrates, large drops form from the rim, and smaller ones form from the bag. "This happens in tens of milliseconds—much slower than anyone expected," says Nakafuji. "Previously, it was observed that such bag breakup would occur in hundreds of microseconds to 1 millisecond, tops."

ALPHA Goes with the Flow

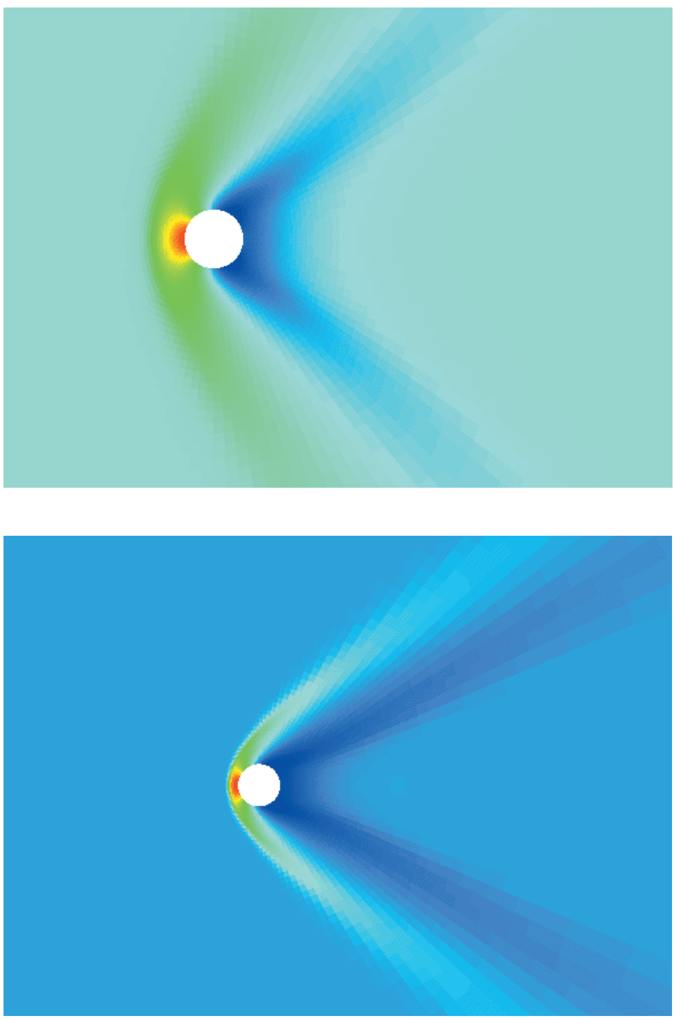
These experiments were conducted in the ALPHA facility, a one-of-a-kind experimental system designed and built by the Livermore–UC Santa Barbara collaboration to examine liquid





(a) The ALPHA facility is a one-of-a-kind experimental system to examine liquid fragmentation. (b) A diagram of the vertical wind tunnel used to re-create a drop falling through the upper layers of the atmosphere.

fragmentation. The facility is essentially a large, vertical wind tunnel, consisting of a cylinder about 3 meters long and 10 centimeters in diameter, that can be pumped down to pressures of 10 to 30,000 pascals. The methodology for re-creating a drop falling through the upper layers of the atmosphere is as follows. An injector releases liquid through a laser beam. The drop breaks the beam, which makes it act like an optical trigger and causes a diaphragm to burst. Air rushes up the cylinder past the drop, in effect simulating the fall of the drop through the atmosphere, and a high-speed camera records the behavior of the drop. "We have the capability to get air moving at velocities of Mach 5—about 1.5 kilometers per second," says Nakafuji. The air flows past the drop at a nearly constant velocity for about 200 milliseconds before its speed begins to ebb, long enough to watch a drop fall, reverse direction, rise, and then burst. This past spring, the group tested a drop 1.5 centimeters in diameter—the largest drop yet tested anywhere. "We don't test actual agents," Nakafuji emphasized. "We use glycerin and other kinds of fluid, and extrapolate to agents from there."



Simulations with Livermore's ALE3D code, which can predict the drag on rigid spheres in subsonic and supersonic rarefied flows, validate a surface-tension model, and test a deformable drop simulation.

Besides examining whether assumptions made at sea level about the breakup of liquid hold true in rarefied environments, the team is also exploring the different break-up modes and whether the dynamics of these modes differ from the dynamics seen for bag breakup. The researchers' efforts have been rewarded. They have documented dynamics that have never before been seen or predicted. "For instance, before the bag breaks, it oscillates at some frequency," explains Nakafuji. "What we saw for the first time—and which no one had expected—is that after the drop turns and begins to move upward, the oscillation frequency doubles. We are now trying to understand this."

Getting Details, Drop by Drop

Ultimately, the team would like to understand and be able to predict the dynamics of specific liquid drops in any rarefied environment. "We'd like to be able to calculate the onset of breakup—when a drop will break up, the configuration the liquid will take, which drops are stable, and which are not," says Nakafuji, adding, "We've definitely made strides in that direction, to the point where we can now accurately predict whether a drop will break up under certain conditions."

The present goal is to obtain critical hydrodynamics and chemical data to validate computer models of these simulations. Working toward this end, the researchers have successfully used the Laboratory's ALE3D code to predict the drag on rigid spheres in subsonic and supersonic rarefied flows, validate a surface-tension model, and test a deformable drop simulation.

"Using experiments and simulations, we are pinpointing the ranges of drop stability and getting a better handle on the physics of liquid breakup," explains Nakafuji. "In the final analysis, we want to be able to predict the rarefied atmospheric conditions under which a given chemical agent will break up into lethal-sized stable droplets. This is a critical question, one whose answer could affect us all."

—Ann Parker

Key Words: ALE3D, ALPH facility, biological agent, chemical agent, lethality, liquid breakup, nerve agent, rarefied atmosphere.

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